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Γ-X interference effects on quasi-bound-state lifetimes in GaAs/AlAs double-barrier heterostructures

D. Z.-Y. Ting and T. C. McGill
Thomas J. Watson, Sr., Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125

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The effect of Γ-X mixing on electron quasi-bound-state lifetimes in GaAs/AlAs symmetric double-barrier heterostructures is studied theoretically using an empirical tight-binding band-structure model. It is found that the Γ quasi-bound-state tunneling times can be shortened or lengthened by Γ-X mixing, depending on whether the AlAs barriers consist of an even or odd number of monolayers. This is attributed to the interference between the Γ and X conduction channels in the AlAs barriers.

I. INTRODUCTION

Since negative differential resistance (NDR) in the double-barrier heterostructure (DBH) was originally proposed[1] and demonstrated[2] by Chang, Tsu, and Esaki, there have been extensive investigations aimed at understanding the process of resonant tunneling and at exploiting the electrical properties of DBH for high-speed analog and digital applications. A particularly interesting application of double-barrier resonant tunneling diodes has been found in the area of high-speed oscillators, which has witnessed steady performance improvement.[3–5] Recently, microwave oscillations up to 712 GHz were reported in double-barrier resonant tunneling diodes.[5] An important characteristic of the double-barrier resonant tunneling diodes in high-speed applications is the tunneling time. Brown *et al.* showed that the maximum attainable oscillation frequency and power output in a resonant tunneling diode depend strongly on DBH quasi-bound-state lifetimes, among other factors. A number of researchers[6,7] have measured tunneling escape times of the lowest quasibound states in GaAs quantum wells (hereafter referred to as $\Gamma 1$ states for convenience). These studies examined the barrier-width dependence of the $\Gamma 1$ state tunneling time in structures with relatively wide quantum wells, reporting times as short as 12 ps.[7]

A recent photoluminescence study[8] of a series of double-barrier structures with varying well width offered indirect evidence that the $\Gamma 1$ state tunneling time in structures with narrow wells may be strongly influenced by Γ-X mixing. To demonstrate the effect of Γ-X mixing on the tunneling escape of electrons from GaAs wells, we have performed a calculation comparing the dynamics of tunneling escape processes in wide- and narrow-well GaAs/AlAs double-barrier structures. We use the one-band Wannier orbital model[9] to describe the conduction-band structures of GaAs and AlAs and solve the time-dependent Schrödinger equation to obtain the time evolution of a wave function initially localized in the GaAs quantum well.[10] The initial wave function is chosen to be constant in the GaAs well and zero elsewhere; it therefore contains a large $\Gamma 1$ component, plus smaller contributions from the higher-lying quasibound states. Since the higher quasibound states have shorter lifetimes, the long-term behavior of the wave function reflects the escape process of the $\Gamma 1$ state. Figure 1 shows the time evolution of electron probability densities integrated over the well region and over barrier regions for (a) a wide-well structure and (b) a narrow-well structure. The insets of Fig. 1 shows the conduction-band diagrams, including both the Γ-point and the X-point profiles, and the $\Gamma 1$ levels of the two structures. Note that the X-point profile shows a double-quantum-well configuration, which can accommodate quasibound states of its own. In the wide-well case, the $\Gamma 1$ level is sufficiently low in energy and is largely unaffected by the X-point states. But in the narrow-well case, the $\Gamma 1$ level is comparable in energy to the X-point states, and can interact strongly with them. Figure 1(a) shows the tunneling escape process in the wide-well structure. After the rapid escape of the components associated with the higher-lying quasibound states, the probability density in the well decays exponentially, with the decay time constant corresponding to the $\Gamma 1$ lifetime. The probability density in the barrier region is relatively small throughout the decay process. In contrast, the narrow-well case in Fig. 1(b) shows the probability density oscillating back and forth between the well and barrier regions during the decay process, indicating strong mixing between the $\Gamma 1$ states localized in the GaAs well region and X-point resonances localized in the AlAs barrier regions.

The qualitatively different tunneling escape processes found in the wide- and narrow-well structures suggest that the $\Gamma 1$ state lifetime is strongly affected by Γ-X mixing. Intuitively, we would expect the X-point states to provide additional channels for tunneling escape, and thereby shorten the lifetimes of quasibound states in the Γ-point quantum well. Indirect experimental evidence and preliminary theoretical results[8] indicate that Γ-X mixing can actually increase the $\Gamma 1$ state lifetime. In

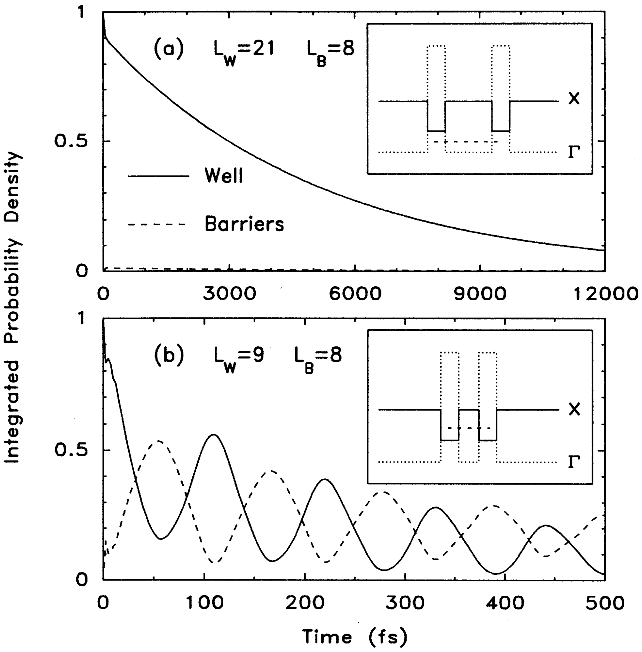

FIG. 1. Time evolution of probability densities integrated over the well (solid curve) and barrier (dashed curve) regions depicting the escape of an electron initially localized in the GaAs well region of a (001) GaAs/AlAs symmetric double-barrier structure. The top panel illustrates the wide-well case (21 monolayer well, 8 monolayer barrier) where Γ-X interaction is insignificant, and the bottom panel illustrates the narrow-well case (9 monolayer well, 8 monolayer barrier) where the influence of Γ-X mixing can be clearly seen. The insets show the conduction-band profiles at the Γ point and the X point for the two structures, with the dashed lines indicating the energy levels of the lowest Γ quasibound states.

this paper, we present a detailed theoretical analysis of Γ-X mixing effects on quasi-bound-state lifetimes in GaAs/AlAs double-barrier heterostructures. In Sec. II we briefly describe our methods. In Sec. III we present our analysis of Γ-X mixing effects on tunneling times. The results are summarized in Sec. IV.

II. METHODS

In our calculation, the energies and lifetimes of quasi-bound states in GaAs/AlAs double-barrier heterostructures are identified by examining the positions and widths of resonances in transmission coefficient spectra. To account for X-point effects, we use an eight-band second-neighbor sp^3 tight-binding model[11] to provide a realistic description of band structures. The Γ- and X-point conduction-band minima energies used in our calculation are shown in Table I. The transmission coefficients are calculated with a numerically efficient and stable method designed to overcome the numerical instabilities[12] frequently encountered in using the transfer-matrix method[13,14] with multiband band-structure models. With this method, the transmission probability can be calculated simply by solving a system of linear equations representing the tight-binding form of the Schrödinger equation over a finite region of interest, with specially formulated boundary and inhomogeneous terms to account for the effects of the incoming and outgoing plane-wave states. A detailed description of the method has been published elsewhere.[15] Quasi-bound-state lifetimes are estimated from the full width at half maximum (FWHM) of the transmission resonances in the transmission spectra using the uncertainty principle

$$\tau \approx \frac{\hbar}{\Delta E_{\mathrm{FWHM}}}. \qquad (1)$$

TABLE I. Conduction-band minima energies (in eV) used in this work.

	Γ	X
GaAs	1.523	1.988
AlAs	2.569	1.654

III. RESULTS AND DISCUSSION

Figure 2 shows the positions of transmission resonances for a series of GaAs/AlAs double-barrier heterostructures with varying GaAs well width and fixed AlAs barrier

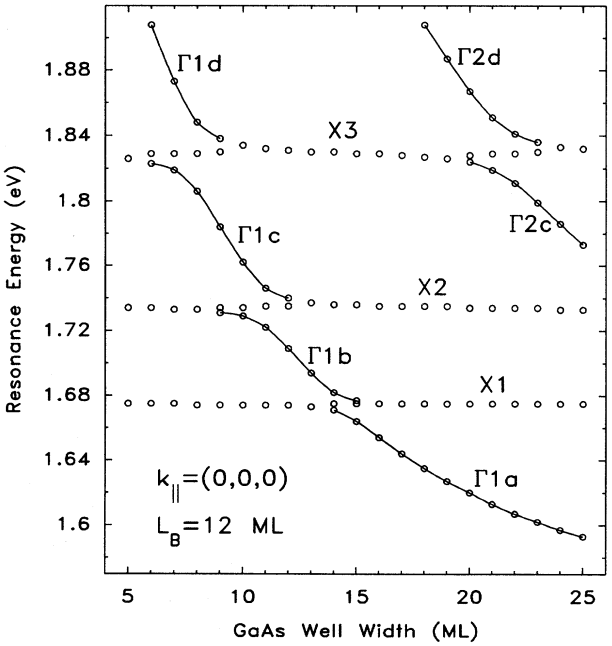

FIG. 2. Positions of conduction-band resonance peaks in GaAs/AlAs symmetric double-barrier heterostructures with GaAs well widths ranging from 5 to 25 monolayers. The AlAs barrier width is fixed at 12 monolayers. The GaAs well Γ-point resonances are connected with solid lines to guide the eye.

width of 12 monolayers. We can classify the resonances by noting that, while the Γ-point resonances decrease in energy with increasing L_W, the positions of X-point resonances should remain essentially constant. We label the resonances by the type of quantum well they belong to (Γ or X) and by their principal quantum numbers. The effect of Γ-X mixing on the quasi-bound-state energy levels is readily seen in this figure. The X-level curves remain relatively constant with changing well width, while the Γ-level curves are broken into separate branches by the X-level curves, forming anticrossing patterns at Γ-X crossovers. To explain this behavior, we use the Γ1-X1 crossover as an example. Recall that there are two X-point quantum wells, each containing a single X1 quasibound state. Since the heterostructure is symmetric, by taking linear combinations of the X1 states in the two X-point wells, we can form a pair of symmetric and antisymmetric states. Normally these two states are nearly degenerate and are seen as a single peak in the transmission spectrum. In the presence of a Γ1 level nearby in energy, the symmetric X1 state interacts with the Γ1 state (which is symmetric) to form two Γ1-X1 mixed quasibound states, yielding two resonances astride the antisymmetric X1 resonance which does not interact with the Γ1 state. In this way, the Γ1-level curve is divided into several branches by the X-level curves; we label them Γ1a, Γ1b, etc. Note that the states with Γ labels can have mixed Γ and X characteristics; they are so labeled for convenience only.

Figure 3 shows the lifetimes of the Γ1a, Γ1b, Γ1c, and Γ1d resonances as functions of the GaAs well width. As before, the barrier width is fixed at 12 monolayers. For comparison, we also computed the Γ1 state lifetimes using a simple two-band model which only includes the Γ-valley band structure of the lowest conduction-band and the light-hole band. The effect of Γ-X mixing on quasi-bound-state tunneling lifetimes can be readily seen by comparing the results from the two models. The two-band model, which does not incorporate Γ-X mixing effects, predicts that the Γ1 resonance lifetime decreases monotonically with GaAs well width. This is as expected, since quasibound states in narrower wells have higher energy and are less confined. Comparing the (eight-band) Γ1a curve with the two-band curve, we note good agreement in the wide-well limit where Γ-X mixing is insignificant. But as the well width narrows to below 18 monolayers where Γ-X mixing becomes important, the Γ1a curve diverges from the two-band curve, predicting considerably shorter tunneling times. The difference may be interpreted as follows: While purely Γ-like quasibound states are confined largely in the GaAs quantum well, the Γ-X mixed quasibound states have wave functions which extend significantly into the AlAs layers. Being less confined, the Γ-X mixed quasibound states have shorter tunneling lifetimes. Similar argument can account for the qualitative behavior of the Γ1b, Γ1c, and Γ1d branches. In particular, we note that each branch shows shorter tunneling times at the two ends than in the middle. This is consistent with our interpretation, since the ends represent states more heavily mixed with the X levels.

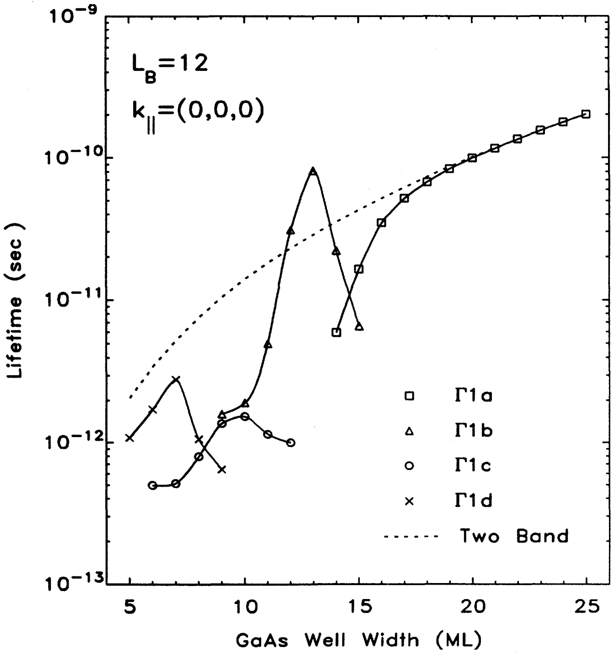

FIG. 3. Lifetimes for the Γ-point $n = 1$, $\mathbf{k}_{\|} = 0$ quasibound states in GaAs/AlAs symmetric double-barrier heterostructures with AlAs barrier width of 12 monolayers, and GaAs well widths ranging from 5 to 25 monolayers. The four branches labeled Γ1a, Γ1b, Γ1c, and Γ1d correspond to the resonances similarly labeled in Fig. 2. Result obtained with a simple two-band model is shown as the dashed line.

In general, the results seen in Fig. 3 agree with what we might expect intuitively, that, by providing additional escape channels, the X-point levels in the AlAs layers enhance the tunneling escape rates of electrons in GaAs quantum-well quasibound states. Although this simple intuitive picture seems to explain Γ-X mixing effects seen in Fig. 3 satisfactorily, we will demonstrate that it can be quite inadequate in certain instances. For example, we note that the points in the middle of the Γ1b branch are actually higher than the two-band curve. Also, a closer examination of Fig. 3 indicates that the Γ1b and Γ1d branches seem rather high relative to the Γ1a and Γ1c branches. Neither of these observations can be explained by the simple picture. The deficiencies of the simple picture are even more apparent in Fig. 4, where we again show the lifetime of Γ1 resonances in double-barrier structures as a function of the GaAs well width. The structures are identical to those shown in the previous example, except that the AlAs barrier width has been changed from 12 to 13 monolayers. Comparing the eight-band and the two-band results, we again note reasonable agreement in the wide well limit. But as we decrease the GaAs well width, the Γ1a curve initially decreases (though at a slower rate than the two-band curve), and then unexpectedly rises to a maximum at $L_W = 16$ before dropping below the two-band curve at $L_W = 14$. At $L_W = 16$, the eight-band lifetime is five time longer than the two-band result. The Γ1b, Γ1c, and Γ1d curves all show tunneling times shorter than predicted by the two-band model. In contrast to Fig. 3, in Fig. 4 the Γ1b and Γ1d branches seem low relative to the Γ1a and Γ1c

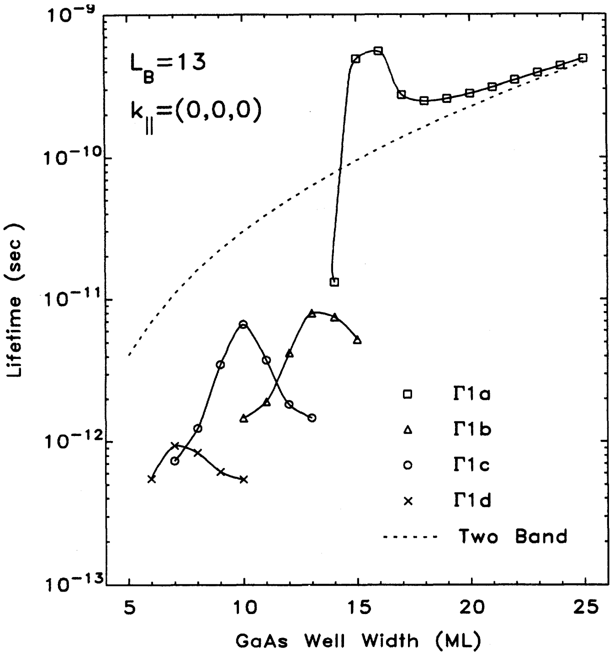

FIG. 4. Lifetimes for the Γ-point $n = 1$ quasibound states. This is similar to Fig. 3, expect that the AlAs barrier width is 13 monolayers in this case.

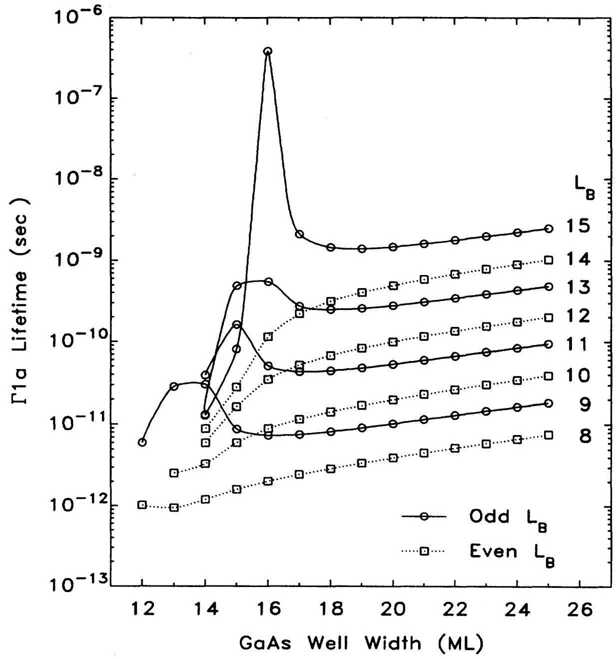

FIG. 5. Lifetimes for the Γ1*a* quasibound states in GaAs/AlAs double-barrier heterostructures as functions well widths for barrier widths ranging from 8 to 15 monolayers.

branches.

The striking difference between the Γ1*a* lifetime curves for the $L_B = 12$ and 13 structures can be seen as a part of a more general pattern. In Fig. 5 we show the Γ1*a* quasi-bound-state lifetimes as functions of well widths, for barrier widths ranging from 8 to 15 monolayers. For the cases shown in this figure, it is evident that while Γ-*X* mixing reduces Γ1*a* lifetimes for structures with even L_B, the opposite is true for structures with odd L_B. These results raise two key questions: (1) We had hypothesized that the additional tunneling channels should increase tunneling rates. How, then, does Γ-*X* mixing increase Γ1*a* quasi-bound-state lifetimes? (2) Why does Γ-*X* mixing have the opposite effects in even-L_B and odd-L_B structures ? We shall try to answer these two questions in the discussions to follow.

We first illustrate how the Γ1*a* resonance lifetime is increased by Γ-*X* mixing. In Figure 6 we show transmission coefficients for a set of double-barrier structures with $L_B = 13$. The well width ranges from 14 to 18 monolayers, corresponding to the cases where the Γ1*a* lifetimes increases are found in Fig. 4. In each plot a dip in the transmission spectrum, known as an antiresonance, is found at $E = 1.661$ eV. In contrast to resonances, which give rise to enhanced transmission, the antiresonances impede transmission. A comparison of Figs. 4 and 6 suggests that the Γ1*a* lifetime increase is caused by the linewidth narrowing in the Γ1*a* resonance as it approaches the antiresonance. This conjecture is supported by the observation (not shown) that there are no corresponding antiresonances in the transmission spectra of double-barrier structures with $L_B = 12$, for which no

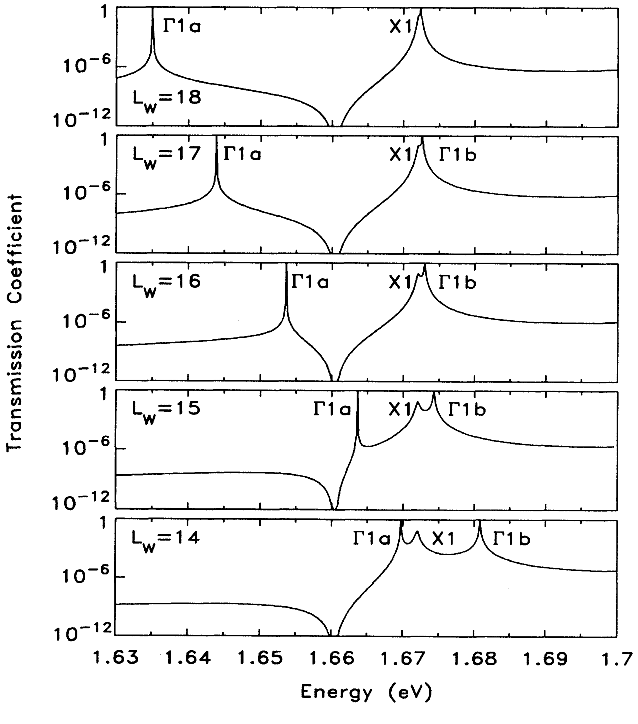

FIG. 6. Transmission coefficients for (001) GaAs/AlAs symmetric double-barrier heterostructures with GaAs well widths ranging from 14 to 18 monolayers. The width of the AlAs barrier L_B is 13 monolayers, and $\mathbf{k}_{\parallel} = 0$.

lifetime increase is found.

The sensitivity of antiresonances to variations in L_B and the insensitivity of antiresonance positions to variations in L_W (see Fig. 6) indicate that antiresonances are associated with the AlAs X-point quantum wells rather than the GaAs Γ-point quantum well. This suggests that we could understand the origin of the antiresonances by focusing on tunneling in the AlAs layers. In Fig. 7 we examine the transmission spectra of GaAs-AlAs-GaAs single-barrier structures with barrier widths ranging from 8 to 12 monolayers, calculated using both the two-band and the eight-band models. The two-band transmission coefficient exhibits the conventional single-barrier tunneling behavior, increasing monotonically with energy. The eight-band spectra show additional resonances and antiresonances due to the presence of the X-point quantum well. Ko and Inkson[16] suggested that the antiresonances may be understood in terms of Fano resonances.[17] A Fano resonance is formed when a discrete level is coupled to continuum states; it is easily recognized by the distinctive asymmetric line shape showing a dip (zero) on one side of the resonance peak (pole). In the GaAs-AlAs-GaAs single-barrier structure, the bound states in the X-point quantum well interact with the continuum of Γ states to form a set of Fano resonances. The antiresonances found in our transmission spectra are in fact the X-point Fano resonance dips. We point out that the Fano resonance asymmetric line shapes are seen frequently in transmission spectra of semiconductor tunnel structures which have multiple tunneling channels. For instance, heavy-hole antiresonances are found in the hole tunneling spectra for GaAs/AlAs double-barrier structures,[18,19] and are attributed to the interference of resonant heavy-hole amplitudes with off-resonant light-hole amplitudes.[18]

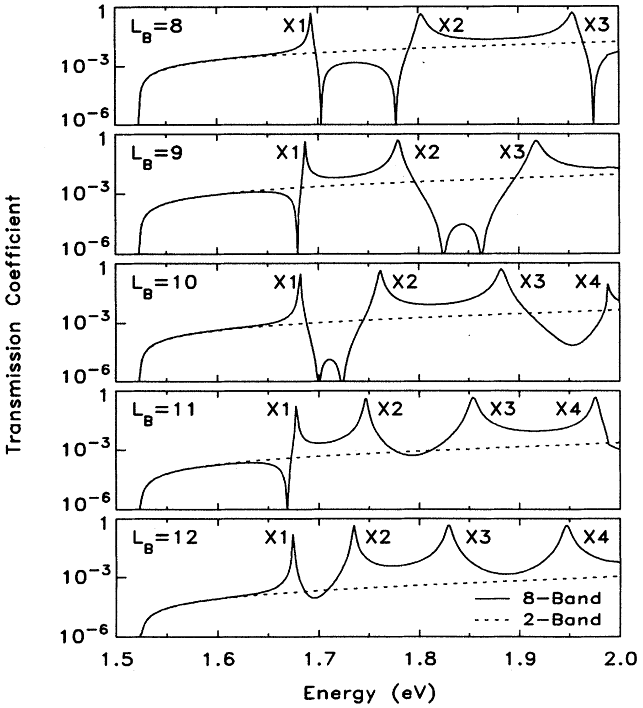

FIG. 7. Transmission coefficients at $\mathbf{k}_\parallel = 0$ for (001) GaAs/AlAs single-barrier heterostructures with AlAs barrier widths ranging from 8 to 12 monolayers. Results obtained with the eight-band tight-binding model and the simple two-band model are shown in solid and dashed lines, respectively.

In the example of the $L_B = 8$ structure shown in Fig. 7, the $X1$ and $X3$ Fano resonances manifest themselves as peaks followed by dips in the transmission spectra, while the $X2$ resonance appears as a dip followed by a peak. Comparing the transmission spectra for the $L_B = 8$ and 9 structures, we note that the sequence of peaks and dips are reversed in the two cases. A systematic study of transmission spectra for L_B ranging from 3 to 40 reveals opposite peak/dip sequences for structures with odd and even L_B's, with the odd-L_B structures showing leading dips and even-L_B structures showing leading peaks. In fact, for $L_B > 10$, resonance peaks are closely spaced, and no antiresonances are found between peaks. Thus the even-L_B structures show no antiresonances at all, and the odd-L_B structures show only the leading $X1$ antiresonances. However, a closer examination of the $L_B = 11$ and 12 transmission spectra in Fig. 7 shows that even though the antiresonances are absent between peaks, the transmission coefficients are still lower between the peaks where antiresonances are expected to be found. For instance, for $L_B = 12$, the valleys are particularly low between $X1$ and $X2$, and between $X3$ and $X4$. This, incidentally, is why the Γ1b and Γ1d branches are high relative to the Γ1a and Γ1c branches in Fig. 3.

Since the lengthening of the Γ1a resonance lifetime in double-barrier structures is caused by the interaction with the leading $X1$ antiresonance, the peculiar L_B dependence of the $X1$ Fano resonance peak/dip ordering is directly responsible for the difference between the Γ1 lifetime curves shown in Figs. 3 and 4. To account for the L_B dependence of the peak/dip ordering of the $X1$ Fano resonance, we made use of the complex conductance analogy by Ko and Inkson.[16] Ko and Inkson showed that the coefficient of the transmitted state t for tunneling through a barrier with multiple tunneling channels may be written as[16]

$$t = \sum_j \alpha_j e^{i(k_j^R + i k_j^I)W} \equiv \sum_j Y_j , \qquad (2)$$

where W is the width of the barrier, k_j^R and k_j^I are the real and imaginary parts of the complex wave vector of the jth tunneling state in the barrier, and α_j depending on the scattering properties of the interfaces; the summation is taken over all exponentially decaying states and forward propagating states. In analogy to parallel circuits, each tunneling channel can be considered as having a complex conductance of Y_j. As in a parallel circuit, both the magnitudes and the phases of the complex conductances are important in determining the total transmission coefficient. In the AlAs barrier, the Γ and X tunneling states in the energy range of interest have purely imaginary and real wave vectors, respectively. Thus, while the Γ-channel phase does not vary with the barrier width, the X-channel phase is barrier-width dependent. To illustrate this dependence, we write a wave vector k

in the X valley as $k = k_0^X + (k - k_0^X) \equiv k_0^X + q$, where k_0^X is the wave vector of the X minimum, and q represents the wave vector k measured from the X minimum. This allows us to write the propagation factor e^{ikW} as the product of a rapidly oscillating term $e^{ik_0^X W}$, which described the consequence of having the conduction minimum located away from the zone center, and a slowing varying term e^{iqW}, which determines the resonance condition in the same way that a Γ-valley propagation factor does (i.e., qW plus phase changes at the interfaces must be integral multiples of π). Assuming the X minimum is at the zone boundary ($k_0^X = 2\pi/a$), and the width of the barrier is L_B monolayers ($W = L_B a/2$), the propagation factor can be written as

$$e^{ikW} = e^{ik_0^X W} e^{iqW} = [(-1)^{L_B}] e^{iqW} = \begin{cases} +e^{iqW} & \text{even } L_B \\ -e^{iqW} & \text{odd } L_B, \end{cases} \tag{3}$$

leading to the following expression for the total conductance:

$$t = \alpha_\Gamma e^{-\kappa_\Gamma W} + [(-1)^{L_B}]\alpha_X e^{iqW} + \cdots \quad . \tag{4}$$

The L_B dependence of the X-channel conductance demonstrated in the equation above results in the qualitatively distinct transmission spectra for even- and odd-L_B structures seen in Fig. 7, and ultimately is responsible for the radically different well-width dependences of $\Gamma 1$ lifetimes seen in Figs. 3 and 4.

We shall end our discussion with a few comments related specifically to the band-structure model used in this calculation. In the empirical tight-binding model, the choice of band-structure parameters is nonunique. Whether odd- or even-L_B structures show leading $X1$ antiresonances can depend on the choice of tight-binding parameters. Schulman[20] has demonstrated that different sets of tight-binding parameters can lead to different peak/dip orderings in the transmission spectrum. We have chosen our parameters such that the lowest conduction-band state at $\mathbf{k} = (0,0,1)(2\pi/a)$ (X point) consists of an anion s-like component and a cation p_z-like component. Also, in our discussions we have assumed that the AlAs conduction-band minimum is located at the zone boundary. The actual AlAs band structure near the X minimum may be a camel's back structure.[21] In that case, the ($k_0^X W$) portion of the X-channel phase would not change by precisely 180° per monolayer; this should lead to some type of "beating" phenomenon as a function of L_B. Nevertheless, for most barrier widths, a monolayer increase should still produce substantial differences in the way that Γ-X mixing affects $\Gamma 1a$ lifetimes.

IV. SUMMARY

We have studied the effect of Γ-X mixing on electron tunneling times in GaAs/AlAs symmetric double-barrier heterostructures using an empirical tight-binding band-structure model. We hypothesized that the X-point states could provide additional channels for tunneling escape from the quantum well, and thereby shorten the lifetimes of Γ-valley quasibound states. However, our analysis indicates that both constructive and destructive interferences can occur between the Γ and X conductance channels in the AlAs barriers, and therefore the lifetime of the $\Gamma 1$ quasibound state can either be lengthened or shortened by Γ-X mixing effects. Specifically, we found that increases in Γ-valley quasi-bound-state lifetimes are caused by the interactions of Γ-valley resonances with X-valley antiresonances. Furthermore, we find that, because the phase of an X-point state changes by 180° degrees per monolayer, the $\Gamma 1$ quasi-bound-state lifetime is either decreased or increased by Γ-X mixing depending on whether the AlAs barriers contain an even or odd number of monolayers.

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